

Dzyaloshinskii-Moriya interaction and magnetic ordering in 1D and 2D at nonzero T

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Abstract –The inclusion of a Dzyaloshinskii-Moriya short range antisymmetric interaction induces spontaneous magnetization, at nonzero temperatures, in one and two dimensions. It is shown that quantum fluctuations are reduced by the Dzyaloshinskii-Moriya interaction, but short range correlations are increased, thereby allowing to obtain long range magnetic order in these low dimensional systems.

Introduction. – In 1966 Mermin and Wagner [1] proved a most relevant theorem, namely that “For one- or two-dimensional Heisenberg systems with isotropic interactions, and such that the interactions are short ranged, namely, which satisfy the condition

$$\sum_{\mathbf{R}} \mathbf{R}^2 |J(\mathbf{R})| < +\infty, \quad (1)$$

there can be no spontaneous ferro- or antiferromagnetic long-range order at $T > 0$.” With only very few rigorous results available this theorem constitutes a most valuable piece of knowledge, especially to test the validity of the usual approximate results. The validity of the theorem was extended, also using the Bogoliubov inequality [2], to classical interacting particles by Mermin [3], and to fermion and boson systems by Hohenberg [4].

In 2001 Bruno [5] extended these results even further, to long range RKKY interactions. More precisely, as formulated by Bruno as a corollary, “A D -dimensional ($D = 1$ or 2) Heisenberg or XY system with interactions monotonically decaying as $|J(\mathbf{R})| \propto R^{-\alpha}$, with $\alpha \geq 2D$, cannot be ferro- or antiferromagnetic.” Physically, it is the fluctuations that prevent the onset of long range order competing against the correlations induced by short range interactions. Therefore, the long range magnetic order observed in one or two dimensional systems could be due, for instance, to magnetic anisotropies or external magnetic fields. In this paper we present an alternative approach, where spontaneous ordering of low dimensional magnetic systems is due to the symmetry breaking that the short range Dzyaloshinskii-Moriya (DM) interaction [6] generates, and which to the best of our knowledge has not been reported in the literature.

The physical basis for the Mermin-Wagner (MW) theorem seems to be the existence of degrees of freedom that are not constrained by an interaction, which makes the fluctuations strong enough to prevent long range order. However, in spite of the fact that the MW theorem excludes the possibility of ordering for a wide range of finite range interactions, we prove below that the Dzyaloshinskii-Moriya (DM) interaction for the Heisenberg Hamiltonian, in spite of being of short range, leads to spontaneous magnetic order in one and two dimensions, at non-zero temperatures. In fact the DM interaction, by reducing the spin fluctuations, yields a canted spin arrangement which turns out to be stable in one and two dimensions.

The Hamiltonian. – The Heisenberg Hamiltonian H_0 , including a weak Zeeman term, is given by

$$H_0 = - \sum_{\mathbf{R}, \mathbf{R}'} J(\mathbf{R} - \mathbf{R}') \mathbf{S}(\mathbf{R}) \cdot \mathbf{S}(\mathbf{R}') - h \sum_{\mathbf{R}} S_z(\mathbf{R}) , \quad (2)$$

where $J(\mathbf{R} - \mathbf{R}')$ is the exchange coupling between atoms located at lattice sites \mathbf{R} and \mathbf{R}' , and h is an external magnetic field parallel to the z -axis. As proved by MW, in the limit $h \rightarrow 0$ and $T \neq 0$ no spontaneous ferro- or antiferromagnetic ordering occurs in 1D and 2D.

The DM interaction can be written as

$$H_{DM} = -2 \sum_{\mathbf{R}, \mathbf{R}'} \mathbf{D}(\mathbf{R} - \mathbf{R}') \cdot [\mathbf{S}(\mathbf{R}) \times \mathbf{S}(\mathbf{R}')] , \quad (3)$$

where the antisymmetric Dzyaloshinskii-Moriya vector \mathbf{D} satisfies $\mathbf{D}(\mathbf{R} - \mathbf{R}') = -\mathbf{D}(\mathbf{R}' - \mathbf{R})$. Therefore, the total Hamiltonian of the system H is

$$H = H_0 + H_{DM} . \quad (4)$$

Method. – We first study the Heisenberg Hamiltonian and later on add the DM term. A convenient procedure to tackle the problem at hand is to use the Bogoliubov inequality in combination with the Fourier transform of the spin $\mathbf{S}(\mathbf{R})$. The latter is given by

$$\mathbf{S}(\mathbf{k}) = \sum_{\mathbf{R}} \mathbf{S}(\mathbf{R}) e^{-i\mathbf{k} \cdot \mathbf{R}} ; \quad \mathbf{S}(\mathbf{R}) = \frac{1}{N} \sum_{\mathbf{k}} \mathbf{S}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{R}} , \quad (5)$$

where the \mathbf{k} sum is limited to the first Brillouin zone.

Let us now consider two operators, A and B whose statistical average does exist. Using the Schwartz inequality for the inner product defined in reference [2], one obtains the following Bogoliubov inequality:

$$\beta \langle \{A, A^\dagger\} \rangle \langle [B, H], B^\dagger \rangle \geq 2 |\langle [B, A] \rangle|^2 , \quad (6)$$

where $\beta = 1/(k_B T)$, $\{C, D\} = CD + DC$ and $[C, D] = CD - DC$.

Defining $A = S_-(-\mathbf{k} - \mathbf{K})$ and $B = S_+(\mathbf{k})$ one obtains, using Eq. (6), for the average spin per site that

$$\begin{aligned} \beta \sum_{\mathbf{k}} \langle \{S_-(-\mathbf{k} - \mathbf{K}), S_+(\mathbf{k} + \mathbf{K})\} \rangle &\geq \\ 2 \sum_{\mathbf{k}} \frac{|\langle [S_+(\mathbf{k}), S_-(-\mathbf{k} - \mathbf{K})] \rangle|^2}{\langle [S_+(\mathbf{k}), H_0], S_-(-\mathbf{k}) \rangle} . \end{aligned} \quad (7)$$

The transverse components are obtained analogously, by defining $A = S_-(-\mathbf{k} - \mathbf{K})$ and $B = S_z(\mathbf{k})$, and using again the Bogoliubov inequality. However, in contrast with the exchange interaction, the DM term yields a spontaneous transverse magnetization, at nonzero temperatures.

Because of translational invariance

$$\sum_{\mathbf{k}} \langle S_i(\mathbf{k}) S_j(-\mathbf{k}) \rangle = N^2 \langle S_i(\mathbf{R}_0) S_j(\mathbf{R}_0) \rangle , \quad (8)$$

and due to the symmetry of the exchange interaction $J(-\mathbf{k}) = J(\mathbf{k})$, Eq. (7) can be written as

$$\frac{\beta s(s+1)}{4s_z^2} \geq \sum_{\mathbf{k}} \frac{1}{\Delta(\mathbf{k})} , \quad (9)$$

where $\Delta(\mathbf{k}) = \langle [S_+(\mathbf{k}), H_0], S_-(-\mathbf{k}) \rangle$ and the spin per particle is $s_z = |\langle S_z(\mathbf{k}) \rangle|/N$. In the continuum limit Eq. (9) takes the form

$$\frac{\rho \beta s(s+1)}{2s_z^2} \geq \left(\frac{k_0}{2\pi} \right)^D \int_{B.Z.} \frac{d\mathbf{u}}{\omega u^2 + h s_z} , \quad (10)$$

where $\omega = s(s+1) \sum_{\mathbf{R}} J(\mathbf{R}) k_0^2 R^2$, $1/\rho$ is the volume per spin, D is the dimensionality of the system, $\mathbf{u} = \mathbf{k}/k_0$ is the normalized momentum and \mathbf{k}_0 is the first Brillouin vector. Since in the limit $h \rightarrow 0$ for $D = 1$ and $D = 2$ the right hand side of Eq. (10) diverges, no spontaneous magnetization occurs at finite temperatures.

Results. – However, if the DM term is taken into consideration, and the full Hamiltonian with finite range interactions given by Eq. (4) is considered, then a spontaneous magnetization does appear. It just leads to the change $\Delta(\mathbf{k}) \rightarrow \Delta(\mathbf{k}) + \Delta_{DM}(\mathbf{k})$, where

$$\Delta_{DM}(\mathbf{k}) = \langle [S_+(\mathbf{k}), H_{DM}], S_-(-\mathbf{k}) \rangle , \quad (11)$$

On the other hand the spin components obey the following inequality:

$$\sum_{\mathbf{k}} \langle S_i(\mathbf{k}) S_j(-\mathbf{k}) \rangle \leq N^2 \langle S_i(\mathbf{R}_0) S_j(\mathbf{R}_0) \rangle , \quad (12)$$

which, combined with $\mathbf{D}(-\mathbf{k}) = \mathbf{D}(\mathbf{k})$ and using $D_{\pm}(\mathbf{R}) = D_y(\mathbf{R}) \pm i D_x(\mathbf{R})$, yields

$$\Delta_{DM}(\mathbf{k}) \leq 2N \left(\frac{\gamma k}{k_0} + \gamma_0 \right) , \quad (13)$$

where

$$\begin{aligned} \gamma &= 4s(s+1) \sum_{\mathbf{R}} |D_z(\mathbf{R})| k_0 R > 0 , \\ \gamma_0 &= 2s(s+1) \sum_{\mathbf{R}} (|D_z(\mathbf{R})| + |D_+(\mathbf{R})|) > 0 . \end{aligned} \quad (14)$$

We notice that, due to the antisymmetry of the DM vector, the first term in Eq. (13) is of order $k = |\mathbf{k}|$, while the exchange term is of order k^2 . This way we obtain, in the continuum limit and with $h \rightarrow 0$, the expression

$$\frac{\rho \beta s(s+1)}{2s_z^2} \geq \left(\frac{k_0}{2\pi} \right)^D \int_{B.Z.} \frac{d\mathbf{u}}{\omega u^2 + \gamma u + \gamma_0} > 0 . \quad (15)$$

If the exchange terms are ignored, which corresponds to the limit $\omega \rightarrow 0$, in one dimension the integration yields

$$\frac{\rho \beta s(s+1)}{2s_z^2} \geq \frac{k_0}{\pi} \frac{\ln(1 + \gamma/\gamma_0)}{\gamma} > 0 . \quad (16)$$

Consequently, infrared divergences ($u \rightarrow 0$) are removed by the DM terms. Moreover, in the $\lim \gamma_0 \rightarrow 0$, *i.e.* when the DM interaction is switched off, the Mermin-Wagner result is recovered, since

$$\frac{\rho\beta s(s+1)}{2s_z^2} \geq \lim_{\gamma \rightarrow 0} \frac{k_0}{\pi} \left[\frac{\ln(1 + \gamma/\gamma_0)}{\gamma} \right] = \frac{k_0}{\pi\gamma_0} , \quad (17)$$

and thus

$$\lim_{\gamma_0 \rightarrow 0} \frac{k_0}{\pi\gamma_0} \rightarrow \infty . \quad (18)$$

However, when the DM interaction is switched on, *i.e.* for $\gamma > 0$ and $\gamma_0 > 0$, the magnitude of the spin per particle is finite, and has both an upper and a lower bound, even in the absence of the exchange interaction

$$\frac{\pi\gamma\rho\beta s(s+1)}{2k_0 \ln(1 + \gamma/\gamma_0)} \geq s_z^2 > 0 , \quad (19)$$

since ρ, β and s are positive.

In two dimensions, in the limit $\omega \rightarrow 0$, we obtain

$$\frac{\rho\beta s(s+1)}{s_z^2} \geq \frac{k_0^2}{\pi} \frac{\gamma - \gamma_0 \ln(1 + \gamma/\gamma_0)}{\gamma^2} > 0 , \quad (20)$$

and by the same token

$$\frac{\pi\gamma^2\rho\beta s(s+1)}{k_0^2(\gamma - \gamma_0 \ln(1 + \gamma/\gamma_0))} \geq s_z^2 > 0 , \quad (21)$$

and we confirmed that the function $\gamma - \gamma_0 \ln(1 + \gamma/\gamma_0)$ is always positive.

Consequently, the DM interaction generates spontaneous magnetic order at nonzero temperature in one and two dimensions.

On the other hand, for the transverse components of the spin we have $\tilde{\Delta}_{DM}(\mathbf{k}) = \langle [S_z(\mathbf{k}), H_{DM}], S_z(-\mathbf{k}) \rangle$. Using the Bogoliubov inequality, in an analogous way to Eq. (13), one obtains $\tilde{\Delta}_{DM}(\mathbf{k}) \leq \omega_0$ with

$$\omega_0 = 4s(s+1) \sum_{\mathbf{R}} |D_+(\mathbf{R})| . \quad (22)$$

Since in the continuum limit the contribution of this constant takes the form

$$\frac{\rho\beta s(s+1)}{s_z^2} \geq \left(\frac{k_0}{2\pi} \right)^D \int_{B.Z.} \frac{d\mathbf{u}}{\omega u^2 + \omega_0} , \quad (23)$$

there is both an upper and a lower bound for the transverse component s_z^2 in one- and two-dimensions, in the limit $\omega \rightarrow 0$, as well.

The DM term Eq. (3), which corresponds to the antisymmetric part of the Moriya tensor [7, 8], and derived from an extension of the Anderson theory of superexchange [9, 10], is linear in the spin-orbit coupling. Hence it represents the leading-order contribution of this interaction. However, as pointed out by Schekhtman *et al.* [11], since the antisymmetric part of the DM interaction $|\mathbf{D}(\mathbf{R} - \mathbf{R}')|$ is of the order of $(\Delta g/g)J(\mathbf{R} - \mathbf{R}')$ and the symmetric one $|\mathbf{\Gamma}(\mathbf{R} - \mathbf{R}')|$ is of the order $(\Delta g/g)^2 J(\mathbf{R} - \mathbf{R}')$, with g the gyromagnetic ratio and Δg the deviation from the free electron value, then

$$|\mathbf{\Gamma}(\mathbf{R} - \mathbf{R}')| \sim |\mathbf{D}(\mathbf{R} - \mathbf{R}')|^2 / J(\mathbf{R} - \mathbf{R}') . \quad (24)$$

and therefore the contribution of the symmetric part also must be taken into account. In addition, performing a local spin rotation in the direction of the antisymmetric DM vector $\hat{\mathbf{d}}(\mathbf{R} - \mathbf{R}') = \mathbf{D}(\mathbf{R} - \mathbf{R}')/|\mathbf{D}(\mathbf{R} - \mathbf{R}')|$, the antisymmetric and symmetric DM interactions can be reduced to an isotropic exchange interaction as shown by Schekhtman et al. [11]. In fact, let us consider an isotropic Heisenberg model with symmetric and antisymmetric components of the DM interaction. The Hamiltonian of this system is given by

$$\begin{aligned} H = & - \sum_{\mathbf{R}, \mathbf{R}'} \left[J(\mathbf{R} - \mathbf{R}') \mathbf{S}(\mathbf{R}) \cdot \mathbf{S}(\mathbf{R}') \right. \\ & + 2\mathbf{D}(\mathbf{R} - \mathbf{R}') \cdot (\mathbf{S}(\mathbf{R}) \times \mathbf{S}(\mathbf{R}')) \\ & \left. + \Gamma(\mathbf{R} - \mathbf{R}') \left(2(\hat{\mathbf{d}} \cdot \mathbf{S}(\mathbf{R}))(\hat{\mathbf{d}} \cdot \mathbf{S}(\mathbf{R}')) - \mathbf{S}(\mathbf{R}) \cdot \mathbf{S}(\mathbf{R}') \right) \right]. \end{aligned} \quad (25)$$

Using a local rotation transformation of the form

$$\begin{aligned} \mathbf{S}(\mathbf{R}) = & (1 - \cos \theta)(\hat{\mathbf{d}} \cdot \tilde{\mathbf{S}}(\mathbf{R}))\hat{\mathbf{d}} \\ & + \cos \theta \tilde{\mathbf{S}}(\mathbf{R}) + \sin \theta \tilde{\mathbf{S}}(\mathbf{R}) \times \hat{\mathbf{d}}, \end{aligned} \quad (26)$$

$$\begin{aligned} \mathbf{S}(\mathbf{R}') = & (1 - \cos \theta)(\hat{\mathbf{d}} \cdot \tilde{\mathbf{S}}(\mathbf{R}'))\hat{\mathbf{d}} \\ & + \cos \theta \tilde{\mathbf{S}}(\mathbf{R}') - \sin \theta \tilde{\mathbf{S}}(\mathbf{R}') \times \hat{\mathbf{d}}, \end{aligned} \quad (27)$$

which correspond to a spin at site $\mathbf{R}(\mathbf{R}')$ rotated around the $\hat{\mathbf{d}}$ axis by the angles θ and $-\theta$, respectively, and where $\sin \theta = D/\sqrt{J^2 + D^2}$ and $\cos \theta = J/\sqrt{J^2 + D^2}$, one obtains

$$H = - \sum_{\mathbf{R}, \mathbf{R}'} \left(J(\mathbf{R} - \mathbf{R}') + \frac{D(\mathbf{R} - \mathbf{R}')}{J(\mathbf{R} - \mathbf{R}')} \right) \tilde{\mathbf{S}}(\mathbf{R}) \cdot \tilde{\mathbf{S}}(\mathbf{R}'). \quad (28)$$

where spin rotated variables preserve the commutation relation,

$$[\tilde{S}_i(\mathbf{R}), \tilde{S}_j(\mathbf{R}')] = i\epsilon_{ijk} \tilde{S}_k(\mathbf{R}) \delta(\mathbf{R} - \mathbf{R}'). \quad (29)$$

The MW theorem establishes that there is no spontaneous symmetry breaking in one and two dimensional systems. This feature is preserved by the DM interaction, since local rotation transformations could be also be defined with opposite chirality ($\theta \rightarrow -\theta$), and hence there is a local chiral invariance underlying the breakdown of rotational symmetry invariance that precludes the spontaneous symmetry breaking. Moreover, Imry and Ma [12] determined that domain formation is energetically favorable against weak random fields, in one and two dimensional systems. And Berezinskii [13] established that in classical systems long range fluctuations develop finite values at large distances. In this sense the magnetic ordering induced by the DM interaction seems to be more closely related to topological ordering, induced some kind of Kosterlitz-Thouless transition [14]. Consequently, the elementary excitations of the system cannot be expanded in terms of standard spin waves.

The DM vector determines the direction of the local rotation of the initial spin variables, and therefore it is possible to find a ground state with a net spin average per particle at finite temperature. However, in spite of the fact that interaction is anisotropic there is no anisotropy energy induced by the DM interaction.

Finally, the terms contributed by the symmetric components of the DM interaction, not included in the exchange interaction, have a constant contribution to the denominators of Eqs. (15) and (23), of the form

$$\tilde{\omega} = s(s+1) \sum_{\mathbf{R}} (|\hat{\Gamma}(\mathbf{R})| + 4|\Gamma_+(\mathbf{R})|), \quad (30)$$

$$\tilde{\omega}_0 = s(s+1) \sum_{\mathbf{R}} |\Gamma_+(\mathbf{R})|, \quad (31)$$

where

$$\Gamma_+(\mathbf{R}) = 4\Gamma(\mathbf{R})\hat{\mathbf{d}}_z\hat{\mathbf{d}}_+ , \quad (32)$$

$$\hat{\Gamma}(\mathbf{R}) = \Gamma(\mathbf{R})(\hat{\mathbf{d}}_+^2 - \hat{\mathbf{d}}_-^2) , \quad (33)$$

$$\hat{\mathbf{d}}_{\pm} = \hat{\mathbf{d}}_x \pm i\hat{\mathbf{d}}_y . \quad (34)$$

Since these terms lift the infrared divergences they induce a net spin per particle in one and two dimensions at finite temperatures.

Conclusion. – In summary, using the Bogoliubov inequality we have demonstrated that a short range antisymmetric or symmetric interaction, as the DM one, generates a long range ordering in low dimensional systems. In spite of the fact that in the ground state there are no coherent long range spin waves, locally the DM interaction induces a small correlation between the spins that reduce quantum fluctuations and induce a net average spin per particle at finite temperature.

In view of the fact that the Mermin-Wagner theorem constitutes an important landmark in the understanding of ordering of magnetic systems which are adequately described by the Heisenberg Hamiltonian, it is significant that the introduction of the Dzyaloshinsky-Moriya interaction [6–8] allows for the stabilization of magnetic order [15] in one and two dimensions at finite temperatures. Furthermore, it also contributes to the understanding of the two dimensional order in layered cuprates, as already pointed out by Kastner et al. [16], and also to understand the stabilization mechanism of two dimensional layers and membranes where long-wavelength fluctuations destroy long-range order.

In closing we underline that i) the DM interaction does not break rotational invariance; ii) the short range order DM interaction does suppress quantum fluctuations in low dimensional systems; and, iii) the particle permutation symmetry of the DM interaction yields contributions to the denominator of Eq. (15), that are of order k^m with $m < 2$, which remove divergences and thus allow for the existence of long range magnetic order in one and two dimensions.

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